

2-Amino-5-nitrobenzanilide

Inchi:	InChI=1S/C13H11N3O3/c14-12-7-6-10(16(18)19)8-11(12)13(17)15-9-4-2-1-3-5-9/h1-8H,
InchiKey:	INKGKPCQLQCFQKB-UHFFFAOYSA-N
Formula:	C13H11N3O3
SMILES:	<chem>Nc1ccc([N+](=O)[O-])cc1C(=O)Nc1ccccc1</chem>
Mol. weight [g/mol]:	257.24
CAS:	30481-54-0

Physical Properties

Property code	Value	Unit	Source
gf	326.61	kJ/mol	Joback Method
hf	102.39	kJ/mol	Joback Method
hfus	39.99	kJ/mol	Joback Method
hvap	90.82	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.429		Crippen Method
mcvol	185.460	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	888.57	K	Joback Method
tc	1159.19	K	Joback Method
tf	643.61	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.30	J/molxK	888.57	Joback Method
cpg	542.28	J/molxK	933.67	Joback Method
cpg	551.16	J/molxK	978.78	Joback Method
cpg	559.05	J/molxK	1023.88	Joback Method
cpg	566.05	J/molxK	1068.99	Joback Method
cpg	572.25	J/molxK	1114.09	Joback Method
cpg	577.75	J/molxK	1159.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30481540&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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